Machine learning-based inverse design methods considering data characteristics and design space size in materials design and manufacturing: a review

Junhyeong Lee[1], Donggeun Park[1], Hugon Lee[1], Kundo Park[1], and Seunghwa Ryu[1,*]

Affiliations

[1]Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

[*]Corresponding author's e-mail: ryush@kaist.ac.kr

Keywords

Artificial intelligence, Inverse design, Machine learning, Deep learning, Data-driven optimization

Abstract

In the last few decades, the influence of machine learning has permeated many areas of science and technology, including the field of material science. This toolkit of statistical methods accelerated the discovery and production of new materials by accurately predicting the complicated physical processes and mechanisms that are not fully described by existing material theories. However, the availability of a growing number of increasingly complex machine learning models confronts us with the question of "which machine learning algorithm to employ.". In this review, we provide a comprehensive review of common machine learning algorithms used for materials design, as well as a guideline for selecting the most appropriate model considering the nature of the design problem. To this end, we classify the material design problems into four categories of: (i) the training data set being sufficiently large to capture the trend of design space (interpolation problem), (ii) a vast design space that cannot be explored thoroughly with the initial training data set alone (extrapolation problem), (iii) multi-fidelity datasets (small accurate dataset and large approximate dataset), and (iv) only a small dataset available. The most successful machine learning-based surrogate models and design approaches will be discussed for each case along with pertinent literature. This review focuses mostly on the use of ML algorithms for the inverse design of complicated composite structures, a topic that has received a lot of attention recently with the rise of additive manufacturing.

1 Introduction

Machine learning (ML) refers to a class of computer-based algorithms in which a user-defined predictive or decision-making machine (surrogate model) improves its own performance by leveraging the sample data, also known as training data. [1]. For the past few decades, ML has been gradually becoming a promising tool in various fields of engineering. Especially, artificial intelligence (AI)-based surrogate models trained by ML can provide a fast and accurate prediction of output for an unknown input configuration, thereby replacing labor-intensive experiments or simulation calculations that demand high computational costs [2-14]. Also, ML-based models can draw meaningful inferences from the given complicated data patterns that humans cannot grasp. For instance, AlphaFold [15] and AlphaGo [16] demonstrated the capability of ML in carrying out remarkable missions that are not conceivable with conventional rule-based computer programs.

With its development, ML also has significantly revolutionized the field of materials design and manufacturing by replacing various classification or regression-related tasks that had been performed by humans. For instance, ML models have performed laborious classification tasks of field experts, such as the detection of abnormalities in manufacturing equipment in real-time [17, 18] and the evaluation of product quality [19-21]. Also, there have been numerous studies on using ML-based regression models to capture the correlation between the design variables of material structures and the resultant performance parameters [22-27]. Furthermore, in recent years, ML has been widely applied to an inverse design of materials and their manufacturing process parameters, encompassing the entire range of a manufacturing process (material development (or selection) – structural design – process parameter optimization) [28-31]. The ML-based data-driven approaches are expected to improve the qualities of production design and production efficiency by suggesting optimal

solutions for complicated inverse design problems even in the absence of prior knowledge about the materials and their manufacturing processes.

The essence of ML-based inverse design is to significantly reduce the cost of generating new data by replacing simulations or experiments with an AI-based surrogate model. In a conventional optimization loop, newly suggested structure designs or process parameter sets are evaluated or labeled by conducting numerical simulations or experiments for every iteration until the optimization process converges to a solution. Therefore, for the optimization problems in which the acquisition of new data is expensive and time-consuming, the surrogate model trained on an accumulated dataset can be extremely beneficial for the optimization task, significantly reducing the costs. For instance, in composite design problems, the elastic properties of various fiber-reinforced composite structures can be computed in a fraction of a second by either analytical theories or simple simulations. With this data acquisition method, either gradient-based optimization or greedy search based on a genetic algorithm can be used for inverse design problems. However, the computation of their non-linear response beyond the elastic regime requires time-consuming simulations or experiments [32]. As another example, the mechanical properties of 3D-printed composites with highly complex geometrical configurations cannot be evaluated simply by analytical models or quick simulations [24, 33]. Thus, for the past few years, the ML-based surrogate model has been extensively utilized to predict and optimize the performance of a new set of composite design problems. For example, starting from the prediction of mechanical properties of comparatively simple-structured fiber-reinforced composites [34, 35], the prediction and design in complex grid composite materials have been studied using ML surrogate models [24, 36].

Despite intensive research and successes in the past years, there still remain challenges in constructing and utilizing AI surrogate models for solving inverse design problems, as

summarized in Table I. First, because of weak generalization performance in an unseen domain, AI models tend to show inaccurate predictions for extrapolation tasks. To find the optimum in a vast design space, exploration of design space outside the initial training dataset is necessary; however, the ML-based prediction model has difficulty in accurately estimating the objective function value of the design that is far from the training dataset [37-43]. Second, although many existing ML-based design studies utilized the data from computer simulations to train ML models due to the ease of accumulating larger datasets, there exists a systematic difference between simulations and experimental results in most cases. Hence, the inverse design based on the trained ML model with the simulation datasets would find the optimum within the manifold of simulation results, which may not represent the realistic optimum. Failure to close the simulation-experiment gap would result in an inaccurate or implausible design, significantly hindering the real-life applicability of the ML-based design algorithms. Finally, the training of deep neural network (DNN) surrogate models generally requires massive amounts of labeled data, which is not always the case in some material design problems [44, 45]. For the cases where simple simulation (or theory)-based prediction is unavailable and high-throughput experiments are difficult to set up, one can only use a small dataset collected through manually conducted material experiments or highly time-consuming simulations, which prohibits the application of deep learning. Therefore, no matter how excellent the emerging DNN architectures are, the predictive performance of the DNN models without sufficient training data may not meet the standards required for an inverse design task. More efficient and practical applications of data-driven optimization can be carried out if one can recognize and overcome the aforementioned challenges.

Table 1. Three challenges in AI-based inverse design problem

Challenges	Methods	Ref. #
Weak generalization performance in an unseen domain	Active transfer learning	[72 – 76]
	Design of DNN architecture	[77]
Difference between simulations and experimental results	Transfer learning	[80 - 82]
Accessible to only small datasets	Bayesian optimization	[76], [87]

This review summarizes different ML-based inverse design frameworks that can be adopted to effectively tackle the materials design problems suffering from the above-mentioned challenges. We classify the inverse design problems into four categories with respect to the size of the dataset and design space, and suggest appropriate design strategies for each case as shown in Figure 1. The first section considers an ideal case in which the design space is relatively small and the dataset is large enough to capture the overall input-output relationship throughout the design space, such that common interpolation-based inverse design schemes can be adopted without concerning the aforementioned challenges (Case 1). The second section considers the design problems that have a vast design space (such as combinatorics or complex shape optimization problems with a high degree of freedom), such that one has to devise a way to mitigate the DNN's weak generalization performance outside the training set (Case 2). Here, an active learning-based gradual ML-model update method or careful design of DNN architecture is suggested to resolve the challenge. The third section highlights the ML-based methods to close the systematic difference gap between simulations and experiments (or between a large low-cost low-fidelity dataset and a small high-cost high-fidelity dataset) (Case 3). A transfer learning or multi-fidelity regression methods are suggested for such case, as the algorithms are capable of incorporating multiple datasets having similar properties. The fourth

section considers the material design problems that have relatively small design space and a small dataset available for the training of a surrogate model, usually due to the objective function being too expensive to evaluate (Case 4). Such design problems can be approached by Bayesian optimization, a sequential design strategy that tries to reach the optimal solution with a minimal number of data acquisition. Finally, the review is closed by describing the ongoing challenges that are yet to be solved, as well as the prospects and future in the field of ML-based materials research.

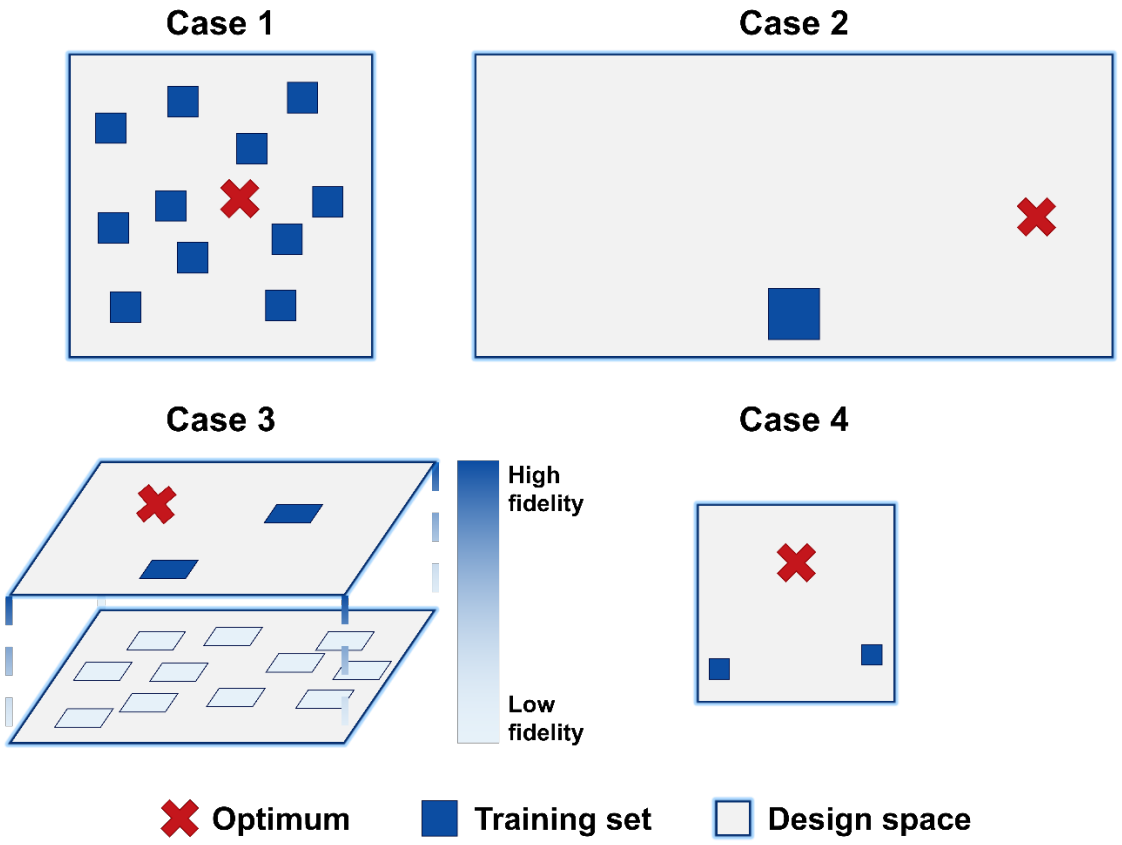

Figure 1. Material design challenges categorized into 4 cases. Case 1: The optimum being near by the initial training region (interpolation), Case 2: The optimum being far from the initial training region (extrapolation), Case 3: Two datasets with different fidelities, and Case 4: A limited amount of dataset.

2 Inverse design using interpolation of AI model (case 1)

ML constructs AI surrogate models that can approximate the output (material performance) as a function of input design variables (structure or process parameters). In particular, deep learning (DL) has enabled a superior prediction compared to conventional ML by using an artificial neural network-based surrogate model that leverages a big data set to learn the complex input-output relationship [24]. The DL-based black-box predictor has allowed researchers to have limited domain knowledge or experience to infer the correlation between the input and the output of a given problem. Many existing studies applied DL to solve various inverse design problems by training a model first and then exploring the optimum in the design space using the trained model [46-50].

In this section, we investigate the case of an inverse design problem in which the optimal design configuration does not deviate significantly from the scope of the initial training set. Here we refer to such case as an interpolation problem. To effectively tackle the interpolation problem, we provide some representative ML-based strategies that are suitable for the case where the amount and reliability of available data are sufficient to describe the input-output relation over the entire design space. For such case, the initially trained ML model generally have an excellent predictive performance over the entire design space, and thus, the optimum design can be found without having to update the ML model during the optimization. Inverse modeling network, forward modeling network combined with a conventional optimization scheme, and a recently emerged generative adversarial network (GAN) will be reviewed in this section.

2.1 Inverse modeling network

An inverse modeling network refers to a neural network trained to predict a design variable as an output while the material performance is given as an input. After training the network, a researcher can use the trained model to determine the optimal values for the design variables by simply entering the desired performance as an input. The method is highly efficient in terms of time as the trained neural network can recommend the optimal designs within a very short time. However, when multiple sets of design variables have identical performance, the training of the neural network for inverse design is difficult as conventional deep neural network models can not effectively capture the one-to-many mapping [51, 52].

Several subsequent studies tried to improve the inverse model approach to overcome the limitation. Kabir et al. (2008) trained an inverse design neural network that predicts the values of geometrical parameters by putting the electrical parameters as input and then used the trained surrogate model for designing microwave guide filters. At first, the study divided the given training data set into different groups in a way that each group does not contain the samples having the same performance but different designs. Then, they constructed multiple inverse modeling networks for each group of training sets, which were later integrated into one form of a comprehensive prediction model. As a result, the proposed method showed higher prediction accuracy than the conventional DNN models that are trained with all training samples at once (Figure 2) [51].

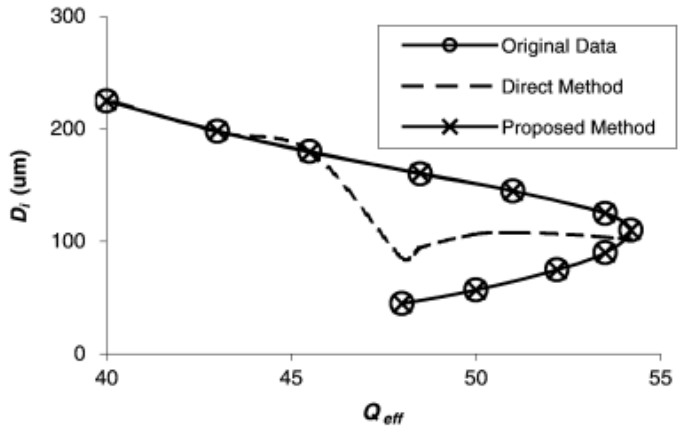

Figure 2. Comparison of the prediction of the inverse modeling network trained by the direct method and the proposed division method for microwave guide filter design [51]

However, although the division method could be readily implemented for the inverse design problems that have a small and simple data structure, division of the training data was far more challenging when it come to a complex design space. Hence, as an alternative solution, Liu et al. (2018) proposed a tandem network architecture, whose structure has an inverse modeling network attached in front of a forward modeling network as described in figure 3. To model the correlation between design and response (performance), the forward modeling network located at the back of the architecture (right side of the figure) is trained first. After fixing the weights trained in the previous step, the remaining inverse modeling network is trained to reduce the error between the predicted response and the desired response. Finally, the trained tandem network was able to generate a design candidate on the intermediate layer M by putting the desired response as an input. Even if there were multiple design solutions for one identical response in the training dataset, the forward modeling network depicting many-to-one mapping was trained accurately. Furthermore, since the inverse modeling of the second training stage did not aim to predict the real design of the train data, the network could be trained effectively despite the data inconsistency. In this study, the proposed tandem-shaped network was applied for the designing of a nanophotonic structure that has the desired performance [52].

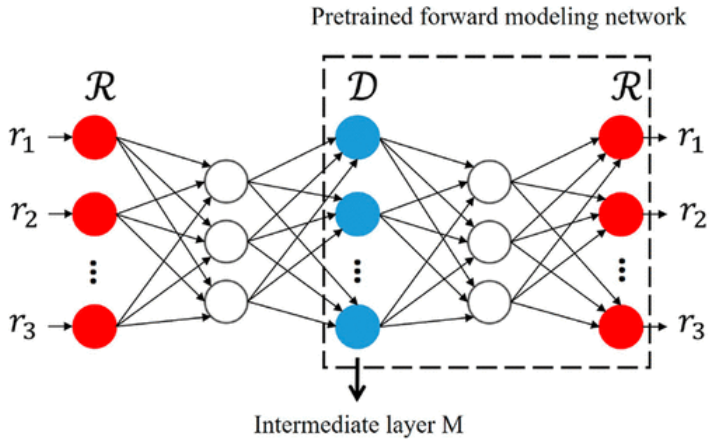

Figure 3. Proposed tandem-shaped neural network for inverse design problem of the nanophotonic structure [52]

Other researches associated with the inverse modeling network include a multivalued neural network for the prediction of multiple output value sets for the same input value, or a network with a unique activation function for smooth learning of the inverse modeling network [53, 54]. The method using the inverse modeling network has the advantage of being able to recommend candidates for the optimal design very quickly once the neural network is trained in simple inverse design problems. However, the dimension of the input variables that correspond to the material performance is usually lower than the dimension of the output variables that correspond to the materials design parameters, thereby limiting the dimension of the recommended optimal values. Such a problem may not be an issue in the case of simple problems in which the dimension of design variables is relatively small, but the strategy may not be applicable for more complex design problems with higher input and output dimensions.

2.2 Forward modeling network + optimization

A forward modeling network, as opposed to an inverse modeling network, is an AI model that predicts the material performance for a given set of design parameters [52]. The forward model has no difficulty in training even if multiple sets of design variables have identical performance values or if the dimension of design variables (input) is much larger than the dimension of performances (output). A well-trained AI model can produce reliable prediction results in a fraction of a second, replacing the time-consuming simulations or experiments that are conducted for the evaluation of objective functions.

In a sequential optimization strategy where the optimization process gradually approaches the global optimum by repeatedly augmenting new data to the model, the acquisition of a new dataset may take a considerable amount of time if numerous iterations of data augmentation are taken. This is especially true when we use computer simulations and experiments that cost significant time to predict the material performance for a given design variable set. Therefore, many studies have been conducted to efficiently find the optimum by combining the AI surrogate model while following the workflow of the existing data-driven optimization algorithm. For instance, Kim et al. (2020) combined the forward modeling network with the conventional genetic algorithm to optimize the structures of an adhesive pillar. In this study, a DNN-based surrogate model is trained with its input being 501 design variables that characterize the 2D shape of an adhesive pillar and its output being the interfacial stress distribution at the boundary between the pillar and a substrate. The stress distribution was compressed into 30 valid features through principal component analysis (PCA) for efficient training of the neural network. The trained neural network was able to predict the output accurately and quickly for 1,000 proposed adhesive pillar designs. Based on the predictive power of the network, the genetic algorithm was performed, and the optimal pillar shapes that can minimize the interfacial stress singularity were found as shown in figure 4 [46]. There are many other studies that performed optimization by combining the forward modeling network

with optimization algorithms such as the genetic algorithm [55] and particle swarm optimization [56].

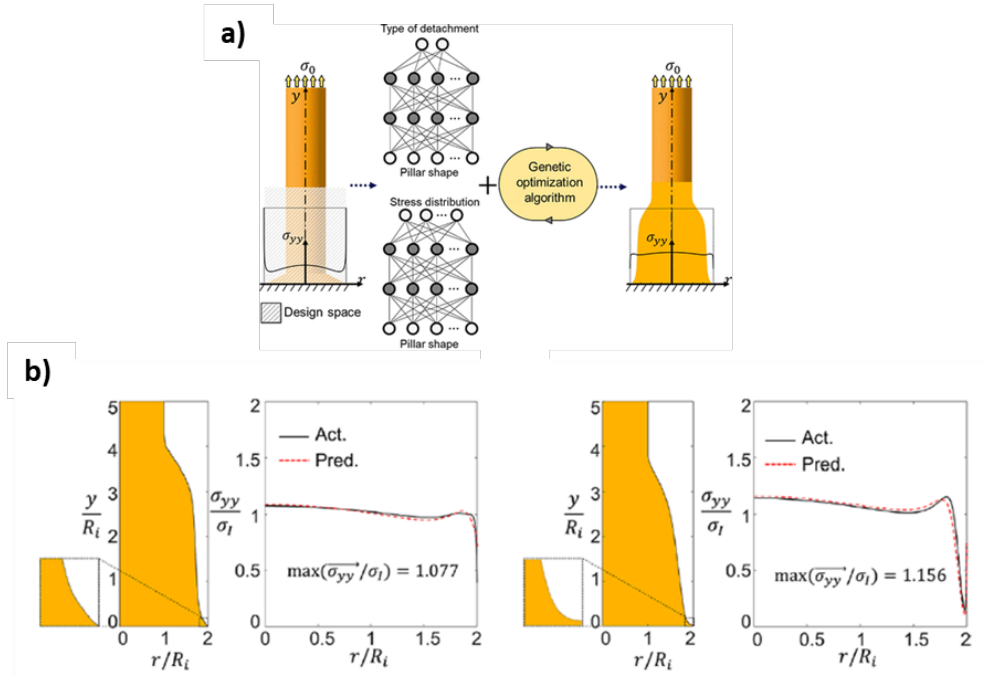

Figure 4. Inverse design of the shape of the adhesive pillar combining the forward modeling network and the genetic algorithm [46]

A different approach called generative inverse design network finds the optimal designs having the desired performance by using back-propagation in neural networks. Generally, back-propagation is a process of optimizing the hyperparameters of hidden layers to minimize the loss function, the value of which quantitatively defines the error between the network's predicted result and the ground truth value [57]. After the training stage, we can find the optimal design by fixing all neural network parameters except for the input features so that the input values are tuned to minimize a loss function through back-propagation.

For example, Peurifoy et al. (2018) solved the inverse design problem using the back-propagation-based approach to find the optimal thickness combination of nano-particle causing

desired light scattering spectrum [58]. First, to construct the AI regression model, the neural network was trained by the data collected from light scattering simulation, which generates the light scattering spectrum for a set of parametrized thickness values of multi-layered nanoparticles. Then, by fixing all weights except for the input features, the optimized particle designs having the desired scattering spectrum were obtained through back-propagation (Figure 5).

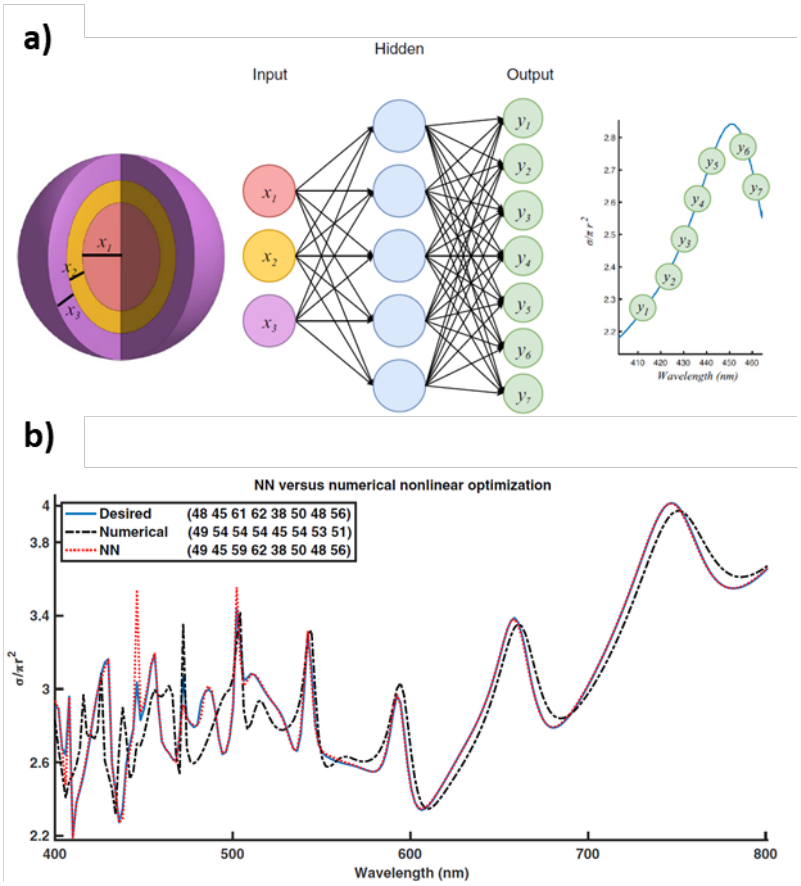

Figure 5. Inverse design of nanoparticles using the forward modeling network and the back-propagation-based optimization method [58]

2.3 Generative Adversarial Network (GAN)

The capability of DL to perform classification tasks further improved the inverse

design framework by classifying whether a new design is realistic or not. GAN (Generative Adversarial Network) is a representative neural network architecture that adversarially trains a generator that creates data and a discriminator that judges whether the created data is similar to the original data set or not, in order to generate new but still reasonable data close to real training data [59]. The GAN has been adopted for research mainly related to image processing [60-62] and it is now rapidly expanding to various applications such as the medical industry [63, 64], natural language processing [65], and voice recognition [66].

GAN has also been employed to solve inverse design problems as it can find a new design candidate with excellent predictive performance, a design that is still similar to the designs within the original training set. Additionally, modified forms of GANs such as conditional GAN (CGAN) [67] and Wasserstein GAN (WGAN) [68] further expanded the scope of inverse design by making the training of the model easier and expanding the types of tasks that the DL can perform.

For example, Kim et al. (2020) applied WGAN to build a network called ZeoGAN and solved the inverse design problem of porous material to obtain the desired level of methane heat of absorption. In WGAN, the discriminator is changed to a critic to quantitatively measure the Earth-mover distance (EMD), which indicates the similarity between the real data and the generated data. The generator is trained to minimize the EMD between the generated data and the original data. In this research, the generator that can create a structure and energy distribution similar to that of porous material from noise input was trained, and the optimal candidates were obtained by modifying the generator's loss function to obtain the desired methane heat of absorption (Figure 6). Since the generator can be trained for other target properties, and the identical framework can be applied to other gases, the expandability of the optimization framework proposed in this research is superb [69].

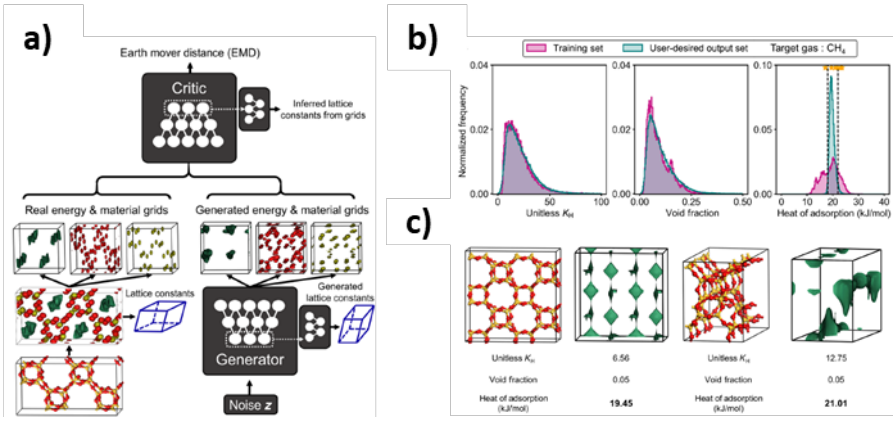

Figure 6. Inverse design of porous material using ZeoGAN [69]

As another example, Yilmaz & German (2020) conducted an Airfoil inverse design study using CGAN. Unlike GAN, CGAN puts a conditional vector during training to limit or to add conditions to the image generated by the generator. In this study, the neural networks were trained to generate only the design of the airfoil shape with the desired stall angle by adding the design range and angle of attack of the aircraft wing as a conditional vector. As a result, various airfoil designs that satisfy the required stall angle condition were successfully obtained (Figure 7) [70].

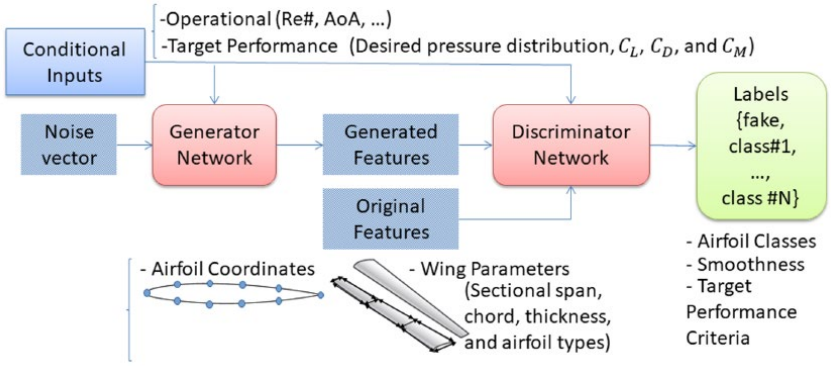

Figure 7. CGAN network to obtain desired airfoil shape design [70]

3 Inverse design requiring extrapolation (case 2)

Recently, the development of manufacturing techniques, such as additive manufacturing, enables the production of materials with very complex topologies, expanding the design space of material structures astronomically. In such humongous design spaces, a randomly generated initial training dataset of average size is usually not informative enough to capture the input-output relationship over the entire design space. Therefore, an extrapolation task has to be performed to explore the design space to find the optimal designs having characteristics significantly different from the initial training set. Although the forward modeling network has high accuracy in predicting the performance of the designs similar to the training data set, the network loses its predictive power when it comes to the unseen design domain far beyond the initial data set [37-43]. Therefore, for the inverse design problem having a vast design space, the extrapolation issue of the neural network should be handled.

The second section introduces AI model-based inverse design methodologies considering a vast design space and extrapolation tasks. The methods can be applied to inverse design problems in which the data has sufficient fidelity, yet the amount is not enough to describe the whole design space. Active learning strategy and novel network architecture will be reviewed in this section to effectively explore the unseen design domain.

3.1 Active transfer learning-based approach

Active learning refers to an ML strategy where the computation model selects the training data by itself and uses it for the training. In addition, active transfer learning is a training method that updates and improves the pre-trained neural network with the dataset selected by the computer itself [71, 72]. Iterative use of active transfer learning can train the neural network so that the model can more accurately predict the performance of the dataset far from the initial training set. Therefore, the deep learning-based optimization framework

based on active transfer learning combined with appropriate new candidate designs provides a clue to the extrapolation challenge in various engineering problems.

For example, Kim et al. (2021) proposed a deep neural network-based forward design framework to explore the unseen design space efficiently. The forward modeling network trained by the initial training dataset showed weak predictive power for the designs that are significantly different from the initial dataset. The proposed method in this study gradually reinforced the deep neural network (DNN) model through active learning by repeatedly training the model with the new candidate designs suggested by greedy sampling and a genetic algorithm. Such a sequential training method allowed the model to propagate toward the optimal designs having excellent mechanical stiffness and strength in the vast design space (Figure 8). The study shows that a new composite design with optimal stiffness and strength can be found in a very efficient way, the size of the augmented dataset being only 0.5% of that of the original dataset. The study also highlighted that the surrogate model must at least have a 'reasonable' extrapolation performance, if the model is to be used for the greedy sampling and genetic algorithm. For example, the DNN model used in this study was trained with the data having low material properties (lower 90%) in terms of stiffness and strength, and the model resultantly showed inevitable prediction errors when it was dealing with the designs having top 10% material properties, as the model was carrying out an extrapolation task. However, although the model was not able to accurately predict the values of stiffness and strength for the designs, the model was capable of determining the relative ranking of the designs by their performance. As a result, the surrogate could be combined with the greedy sampling algorithm and genetic algorithm, together forming the active transfer-learning framework. However, the same approach could not be adopted for the optimization of composite for toughness, which corresponds to the total area under the stress-strain curve, as the DNN model failed to show the minimal predictive power to carry out the ranking of the predicted designs. Insufficient

predictive power can be improved based on domain knowledge from solid mechanics [72].

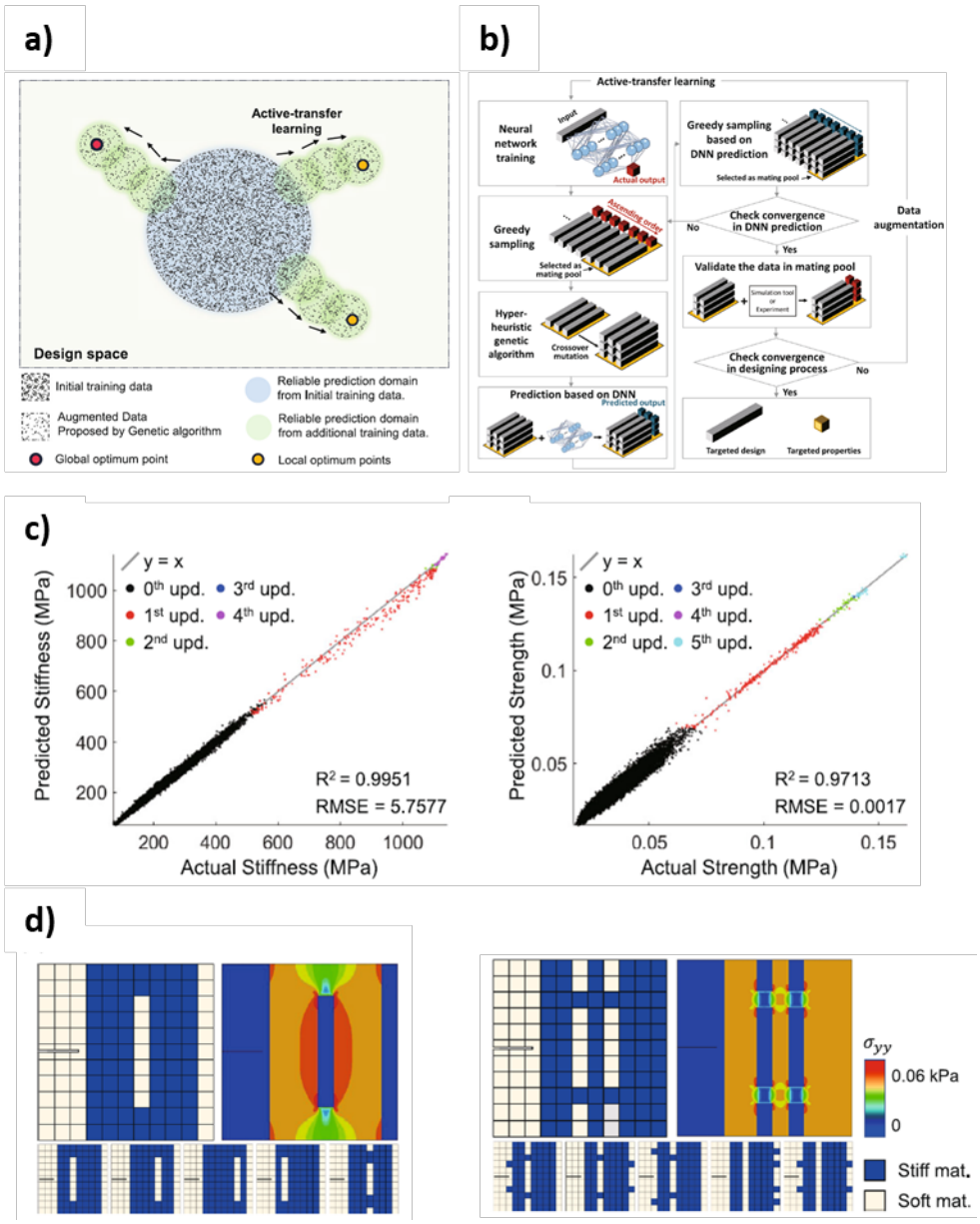

Figure 8. Stiffness and strength optimization of grid composites using active transfer learning and genetic algorithm [72]

The active transfer learning-based framework has been successfully applied to the

optimization of composites and structures for other target properties. Demeke et al. (2022) adopted the active transfer learning-based optimization framework for the inverse designing of a thermoelectric power generator to achieve high power and efficiency (Figure 9) [73]. Lee et al. (2022) found a superb lattice structure with high stiffness and strength by applying the framework to the optimization problem of the density and mechanical properties of the lattice structure constituting the crisscross pattern of beam elements (Figure 10). As above, the adaptive framework has provided a solution to the optimization problem with a myriad of possible shapes [74].

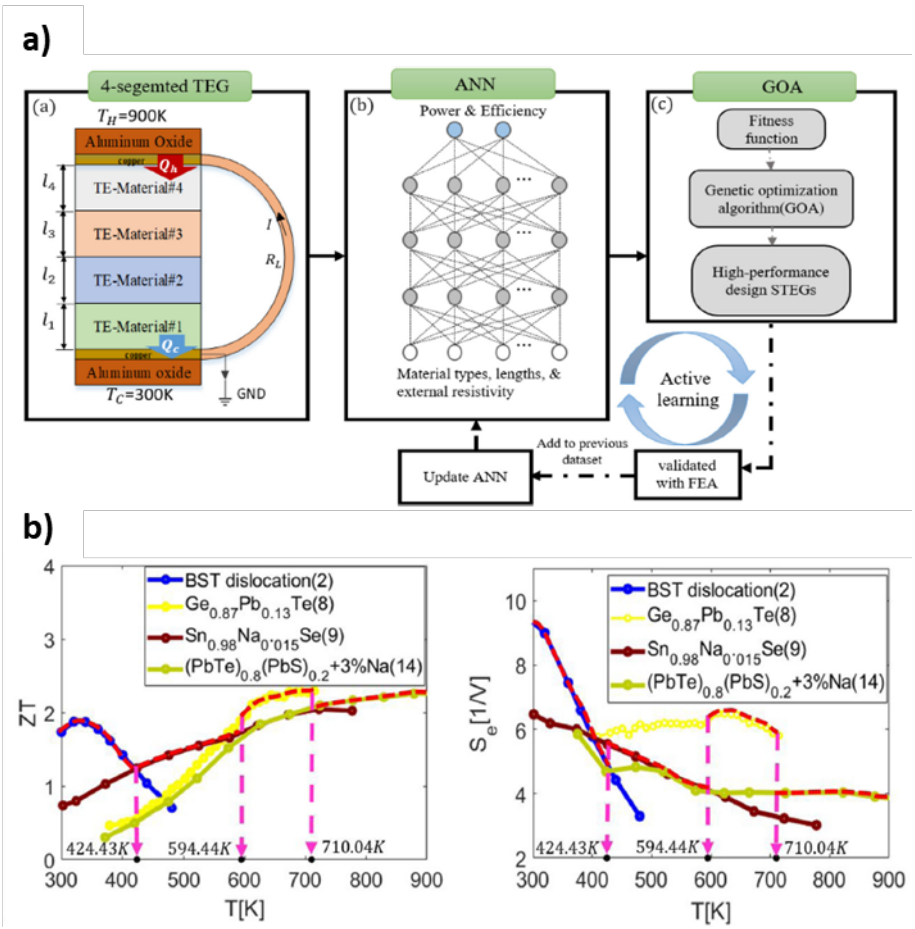

Figure 9. Thermoelectric power generator optimization using active transfer learning and genetic algorithm [73]

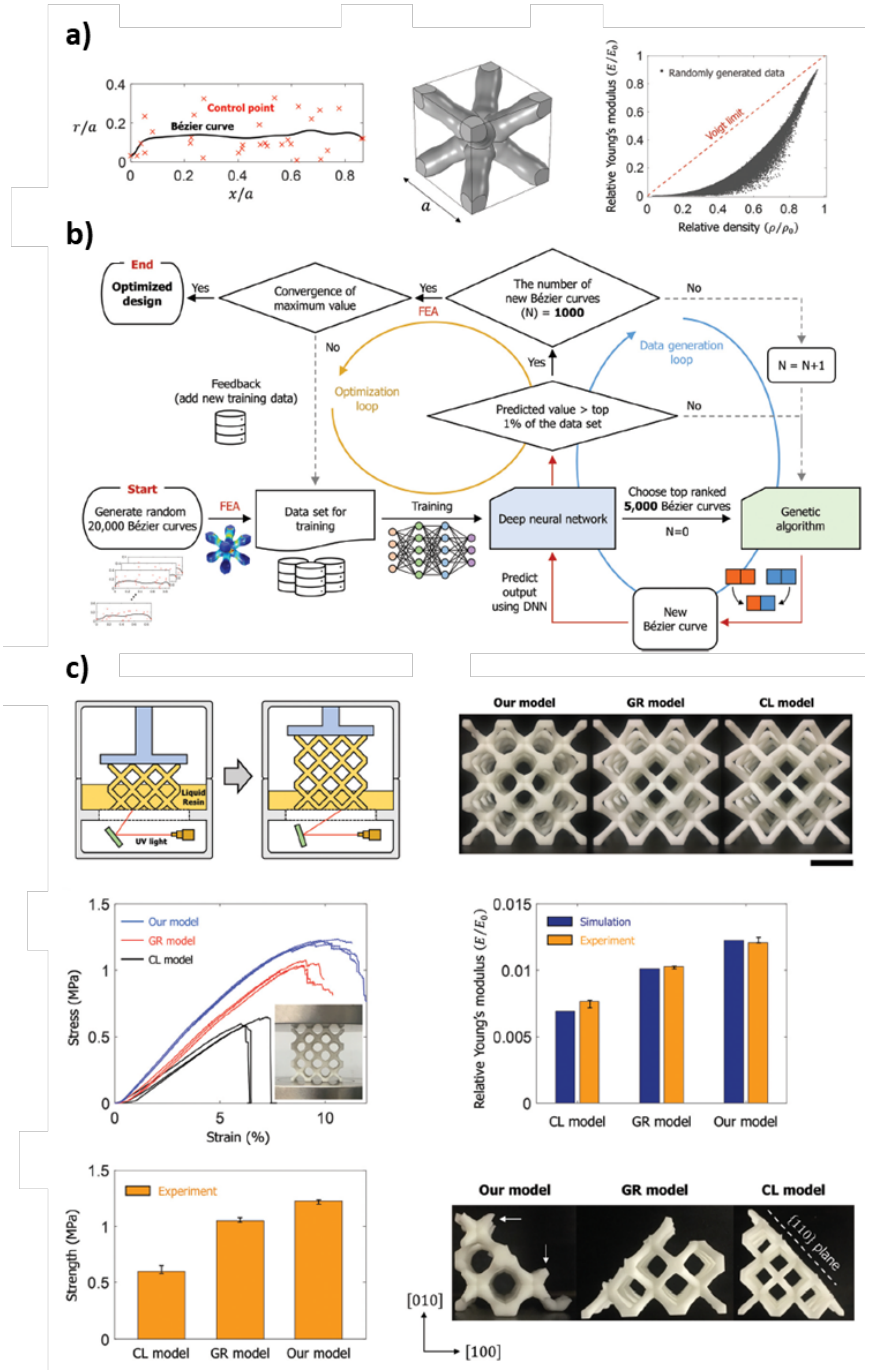

Figure 10. 3D-printed lattice structure optimization using the genetic algorithm aided by active transfer learning [74]

On the other hand, optimization using back-propagation combined with active transfer learning also enables an exploration method toward the wider design. Chen and Gu (2020)

introduced a generative inverse design network (GIDN) framework recommending optimal designs based on back-propagation and active learning. The GIDN framework proceeds in three stages: predictor training, recommendation of optimum based on back-propagation, and active transfer learning. In the predictor training stage, the AI surrogate model that predicts the output performance of an unknown input design is trained with the initial training samples. Next, the desired values are put into the output layer, the weight of the hidden layer is fixed, and the optimal design candidates are recommended using back-propagation. Finally, the study proceeds with active transfer learning, which evaluates the actual performance of the recommended candidates so that the new data set can be used for the updating of the predictor. By iteratively performing the process above, the predictor is gradually updated to have high predictive power for higher-performance designs that are far from the initial training data. This study optimized the geometrical configuration of a grid composite structure, a 2D array of stiff and soft materials ordered in a random manner, to design a higher-toughness composite using the aforementioned inverse materials design method (Figure 11) [75].

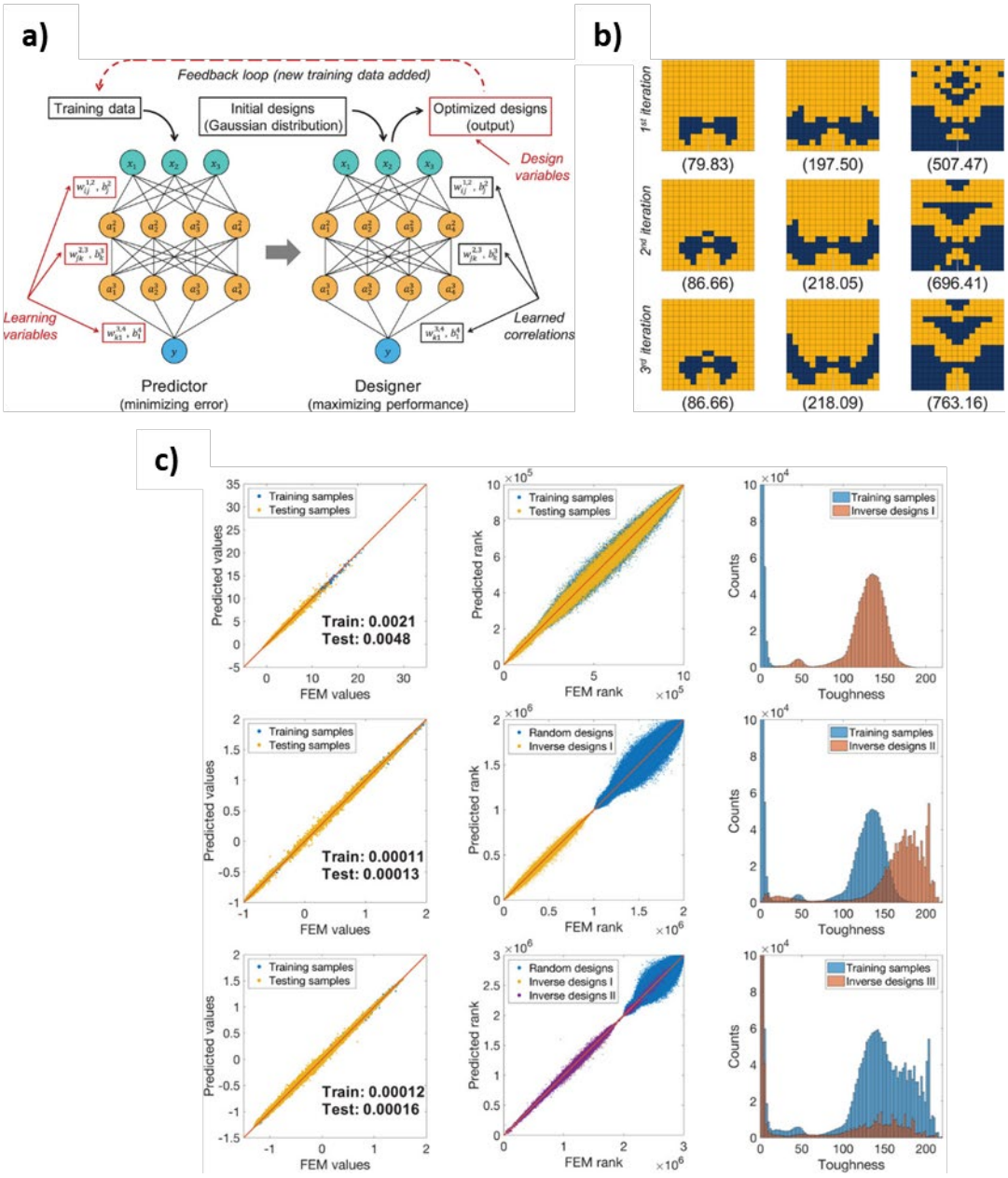

Figure 11. Toughness optimization of grid composites using active learning and back-propagation-based optimization [75]

Furthermore, Jung et al. (2022) proposed a process parameter optimization method for the injection molding process using constrained GIDN (CGIDN). The conventional GIDN has a limitation in that the recommended input design from the desired output is unbounded. The

CGIDN proposed in the study recommends the process parameter set within a desired range by applying a constraint to the input layer via the sigmoid function. As a result, they were able to find the optimal injection molding process parameter set that simultaneously minimizes deflection after injection and the cycle time required for the production [76].

3.2 Extrapolation via improved DNN architecture

As an alternative approach, the extrapolation performance of a DL model can also be significantly improved by devising a better architecture of neural networks. Recently, Park et al. (2022) proposed a modified version of the conventional U-Net architecture that can more accurately conduct the extrapolation task of predicting the stress and strain field in the binary grid composites. As one can deduce the effective mechanical properties of the composite from its stress and strain fields, the proposed DL architecture, having an excellent predictive performance on configurations that are very different from the training set, can be beneficial in searching for the optimal design configurations [77].

Previously, there was a study that applied the conventional U-Net architecture to predict the local stress field for an unknown configuration of the grid composite. U-Net was able to successfully predict the stress/strain field corresponding to the composite constituents by compressing the composite shape spatial information, and supplementing and expanding the compressed information. Yet, U-Net predicts the material local fields without considering various spatial kernel effects and it drops a lot of information from an algorithmic point of view. Hence, it was difficult to guarantee the generalizability of the model for a vast design space, indicating that U-Net still has limitations in making the predictions for a grid composite structure that is very different from the training datasets, in terms of the relative volume fraction (VF) of the two constituent materials [78].

Park et al. (2022) approached the problem by redesigning the DNN architecture to better predict the strain field in the unseen VF domain. This study used a multi-kernel methodology to efficiently extract the composite configuration-strain field relationship in various scales, and proposed a DNN architecture that continuously reuses the extracted information. The proposed network architecture successfully predicted the strain field of the grid composite structure that has a VF that is significantly different from the designs in the training set. In addition, this modified model showed the equivalent predictive performance even with a data set 1/3 times smaller than that used for the existing model. This research clearly showed that one can redesign the DNN architecture to efficiently tackle the purpose of the optimization problem. Here, the modified network exhibited an excellent extrapolation performance near the optimal design even without the sequential active learning process introduced in the previous section. We foresee more research works toward new DNN architecture design in the material/structure optimization field to enable faster and more efficient search for the optimal materials design outside the initial training set.

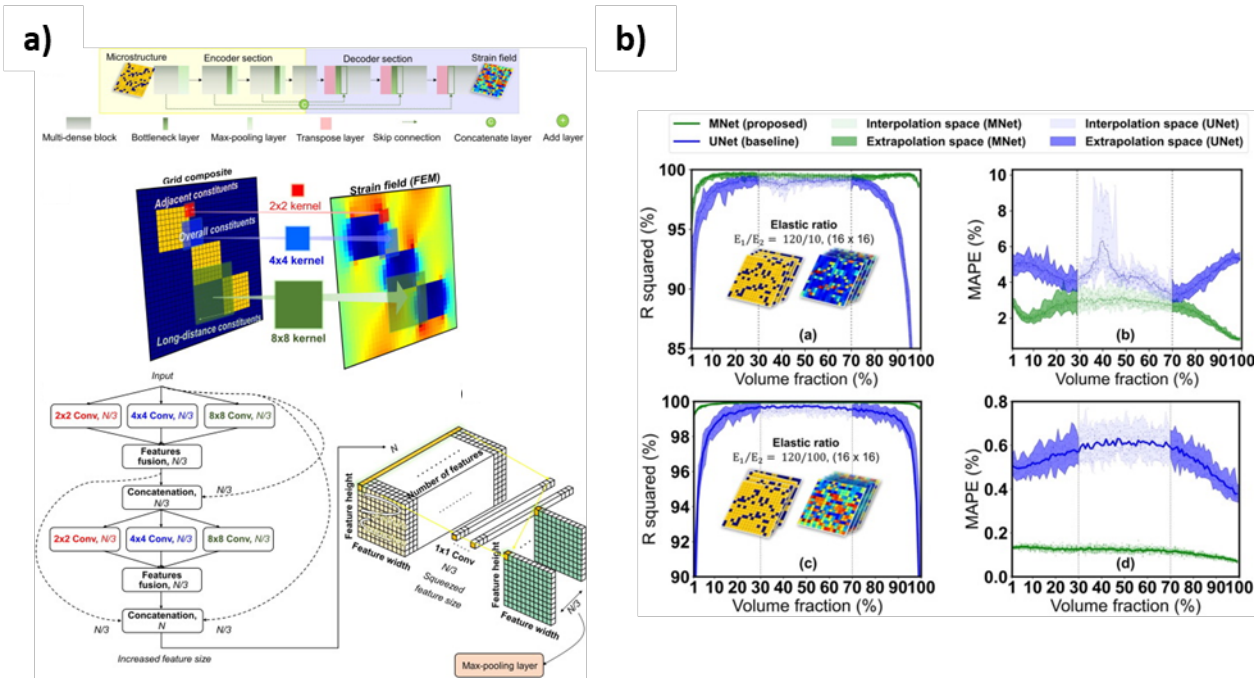

Figure 12. Multi-filter CNN architecture predicting stress field of the grid composite and its

extrapolation ability [77]

4 Inverse design with two different data sets (case 3)

This section deals with the data-driven design method in the presence of two datasets with different fidelities. In particular, we focus on the training scheme for DNN when a big low-fidelity dataset (easily evaluated) and a small high-fidelity dataset (expensive to evaluate) coexist. We introduce the concept of transfer learning and how the transfer learning can be used to construct a DNN-based surrogate model that can make the prediction at the fidelity level of the small accurate dataset. Once the DNN model is constructed, one can adapt the optimization frameworks introduced in section 3. Some examples of solving the inverse design problem using a surrogate model built by transfer learning will also be introduced.

4.1 AI surrogate model using transfer learning

Transfer learning is a strategy to construct a neural network to learn input-output correlations of the desired dataset (typically, a small dataset with high fidelity) by using the dataset to perform fine-tuning of a pre-trained network, which is initially trained with a preliminary dataset (typically, a big dataset with low fidelity). The fine-tuning process of the transfer learning refers to either selecting only a few hidden layers from the pre-trained neural network for the training, or slightly modifying the overall weights in a reduced learning rate and epoch. Hence, if a pre-trained model exists for a similar task (that pertains to the preliminary dataset), it is easier to develop a surrogate model of our interest, as the fine-tuning of the pre-trained model generally requires a dataset of relatively small size. Owing to this advantage, the transfer learning drew big attention particularly in the research fields that have multiple sources of data, one domain where data can be easily collected and another domain where data acquisition is difficult. [79]

For example, Xu et al. (2021) applied the transfer learning technique in building an AI surrogate model that predicts the material properties of grid composites from the microstructure of composites. At first, the study developed a pre-trained CNN model that predicts the statistical parameters for a given grid configuration, which pertains to a problem whose input-output data can be computed relatively easily. After that, the pre-trained CNN was fine-tuned by the small number of FEM datasets so that the final model can predict the effective elastic modulus of the composite. By using transfer learning, it was possible to reduce the amount of FEM data for CNN training by half (Figure 13) [80].

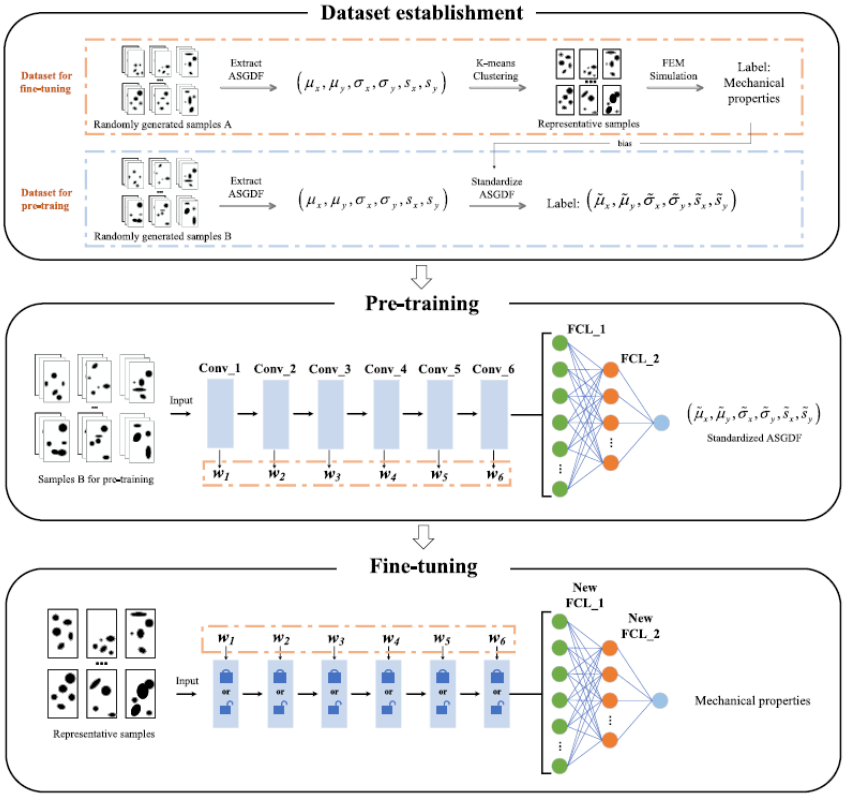

Figure 13. Transfer learning workflow for micro structure-property prediction using CNN [80]

As another example, Jung et al. (2022) used the transfer learning technique to predict

the non-linear mechanical responses of fiber-reinforced composites. The mean field homogenization technique can quickly compute the non-linear mechanical response beyond yield for the composites containing ellipsoidal reinforcement based on a few theoretical assumptions. However, if the shape of the reinforcement is not ellipsoidal or the volume fraction of the reinforcement material is higher than 20%, the prediction accuracy drops significantly. In contrast, although it demands higher computational cost and time, the finite element method (FEM) based calculations with fine mesh provide data of higher accuracy compared to that computed with the homogenization theory. This study pre-trained the DNN using the big homogenization-based data, and then fine-tuned the DNN with the high-accuracy FEM dataset. As a result, the constructed DNN could accurately predict the elastoplastic response of unknown composite geometries. The transfer-learned AI model showed higher prediction accuracy than a DNN trained only using FEM data (Figure 14) [81].

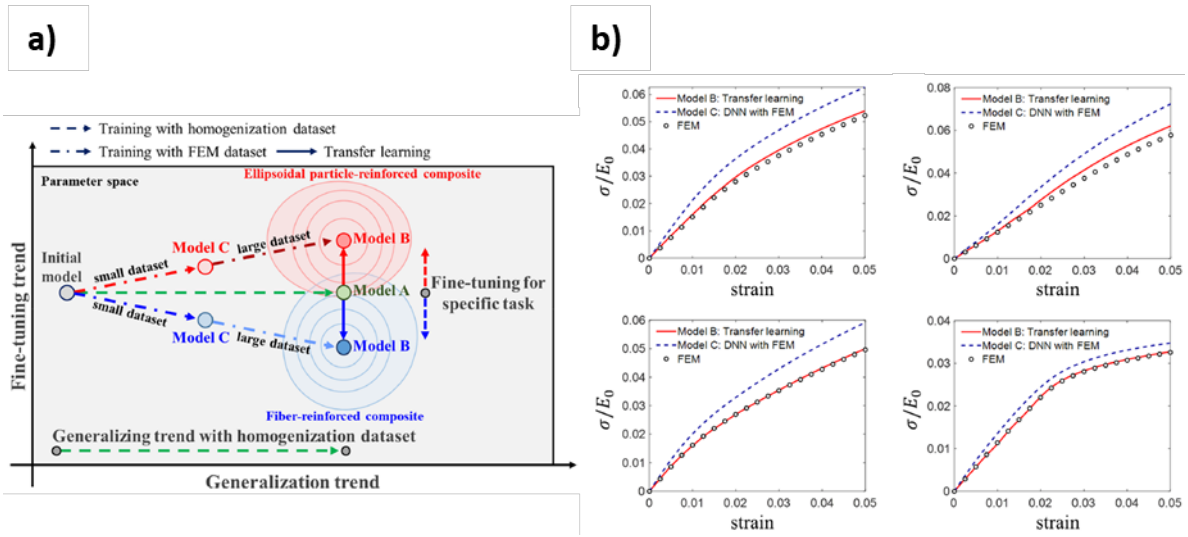

Figure 14. Prediction of elastoplastic behavior of fiber-reinforced composites using the transfer-learned DNN model [81]

4.2 Inverse design using transfer-learned AI model

The DNN-based surrogate model obtained by transfer learning can be combined with an appropriate optimization algorithm to solve the inverse design problem. For instance, Dong et al. (2021) combined a DNN-based surrogate model constructed by transfer learning with conventional data-driven optimization algorithms such as genetic algorithms and Bayesian optimization to inverse-design an optical material (composite metal oxides) having desired light absorption spectrum. To be specific, the purpose of the study is to find a mole ratio of a listed material composition that results in the desired absorption spectrum. The challenge lies in the training of an AI model as a relatively small number of data was available for the materials in the list. To overcome this hurdle, the researchers pre-trained the initial model with a large pool of available datasets, although their material compositions are different from the materials of their interest. After that, they fine-tuned the pre-trained model with a small number of data having the material compositions of their interest. As a result, they were able to construct a surrogate model that can predict the absorption spectrum based on the mole ratio of its material composition. Then, the genetic algorithm and Bayesian optimization were carried out with the transfer-learned surrogate model to discover the optimal design (Figure 15) [82].

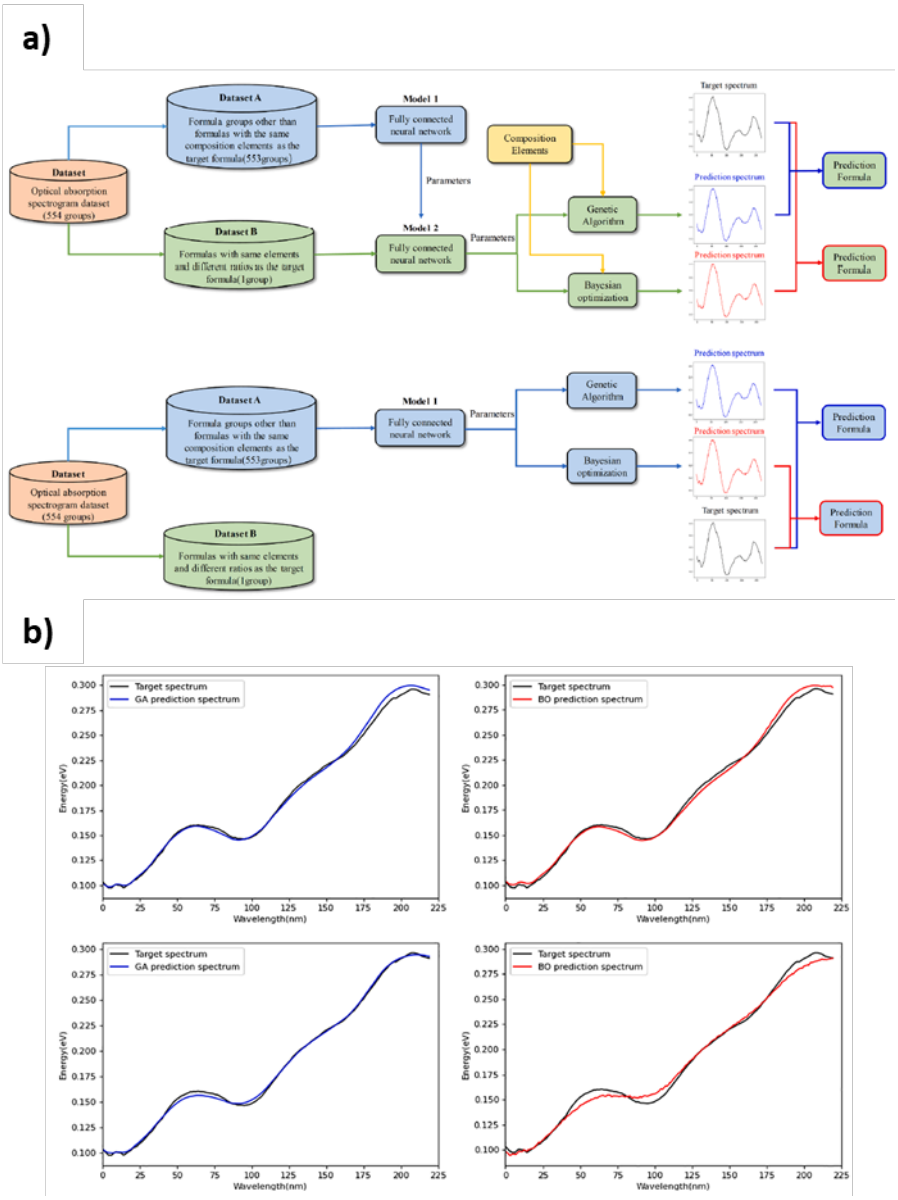

Figure 15. a) overall flow of optimization using AI surrogate model constructed by transfer learning, b) result of optimization of mole ratio of composite metal oxides [82]

5 Inverse design with inaccurate and small data sets (case 4)

In this section, we introduce data-driven inverse design methodologies applicable under the presence of a small dataset, obtained through time-consuming experiments or heavy simulations. Under a scarcity of training data, it is difficult to build a DL-based surrogate model, as they generally require a massive amount of training data for the modeling of a complex input-output relationship. The DL-based algorithms introduced in the previous sections generally had two process components; the construction of an AI-based surrogate model followed by the actual optimization process based on appropriate optimization algorithms. In this section, we review a data-driven method that simultaneously explores the design space and searches for the optimal design.

5.1 Gaussian process regression combined with Bayesian optimization

Bayesian optimization (BO) is a widely used data-driven optimization method that has the advantage of finding the optimum when only a small amount of data is available, due to the cost of data acquisition being too expensive, and the size of the design space being relatively small. Unlike gradient-based optimization, BO repeatedly recommends a new candidate design based on the 'acquisition function', which simultaneously considers the characteristic of exploitation (i.e. searches the region close to the optimum) and the exploration (i.e. searches for the region with large uncertainty in the regression model). Therefore, BO requires a regression model that can quantitatively estimate the expected value and the confidence interval of the expectation simultaneously [83].

Gaussian process regression (GPR) is a representative regression methodology that can estimate the predicted value and its reliability at the same time [84]. GPR assumes that the

data points follow a multivariate Gaussian distribution, and defines a covariance function between the data points to calculate the mean which corresponds to the prediction value at an input data point, and the standard deviation which indicates the reliability of the prediction. The BO algorithm then computes the 'acquisition function' of various design candidates based on the mean and the variance estimated by GPR, and the design that has the highest acquisition function value is recommended as the design to be evaluated next. The expected improvement function, one of the most well-known acquisition functions, is calculated as a weighted summation of the exploitation part, which is related to finding a value close to the optimum, and the exploration part, which is related to the uncertainty of the model. The expected improvement function with an appropriate balance between exploration and exploitation should be used in order to effectively approach to the global optimum [85, 86].

Recently, Park et al. (2022) adopted BO to optimize the toughness of staggered platelet composite structure, which is one of the representative biomimetic composite structures mimicking a nacre. This composite material has a structure in which a stiff material is placed in a brick form on a soft polymer matrix. Because the prediction accuracy of toughness from either analytical models or computer simulations is not satisfactory, authors collected the toughness data by using a 3D printer to build an actual composite and conduct uniaxial tensile tests. With this accurate, yet expensive-to-evaluate, data collection method, they designed the maximum-toughness structure via Bayesian optimization with a relatively small number of experiments. The results from the study are visualized in Figure 16 [87].

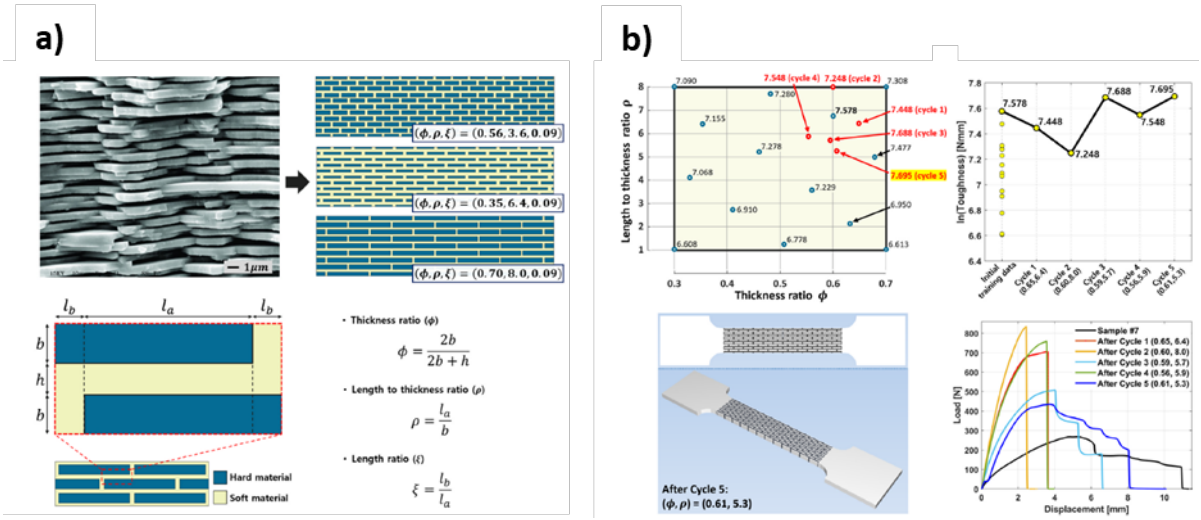

Figure 16. Staggered platelet composite structure optimization using the Bayesian optimization framework [87]

BO can be also extended to solve problems involving multiple objective functions. Multi-objective Bayesian optimization (MBO) aims to find Pareto optimal solutions for multiple objective functions in a trade-off relationship (such as toughness and strength for structural materials, production speed and defective rate for a manufacturing process) [88, 89]. Recently, several studies in materials design and manufacturing adopted MBO to solve inverse design problems with multiple objectives. For example, Jung et al. (2022) applied MBO to optimize the injection molding process parameters and were able to determine the Pareto-optimal process conditions that minimize both the cycle time to produce a single product and the deflection that occurs after production (Figure 17) [76].

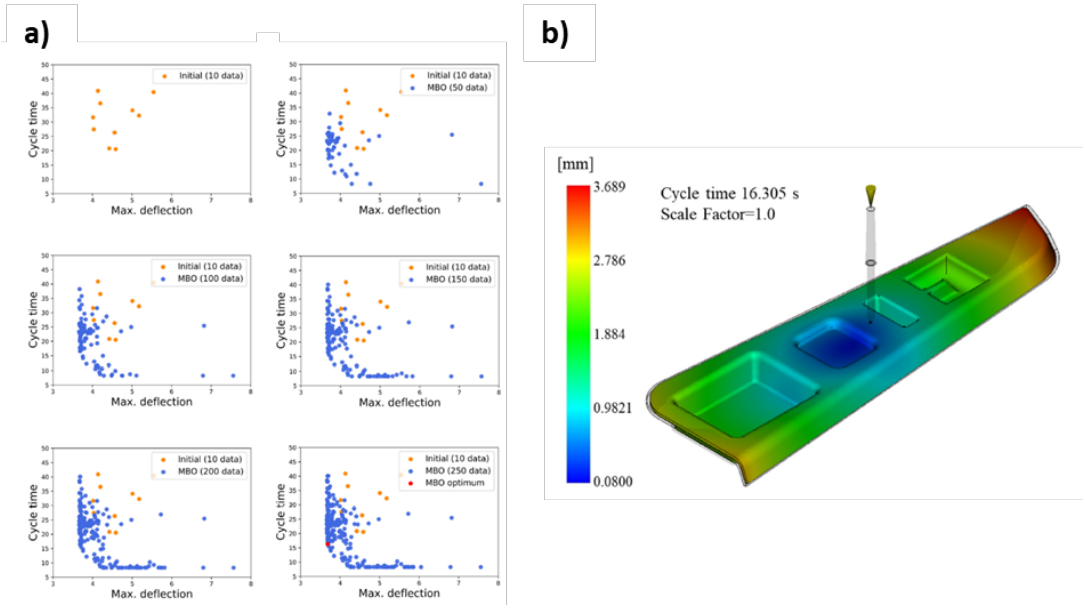

Figure 17. Process parameter optimization of injection molding using Multi-objective Bayesian optimization [76]

6 Conclusion

The advancement of machine learning enables fast and accurate classification and regression for the dataset in the field of materials design and manufacturing. Furthermore, conventional inverse design approaches that rely heavily on people's knowledge and experience can be revolutionized by making the best use of the accumulated dataset through data-driven design methods. A variety of fast and efficient AI model-based algorithms have been proposed over the last few decades and facilitated complex material optimizations even without domain knowledge. However, each of the proposed ML-based methods has its own unique strengths and weaknesses, leaving us with a fundamental question of ‘which machine learning algorithm to choose’.

This review categorizes several ML-based optimization methodologies according to their characteristics of trainable data and the size of the design space. First, in a case where sufficiently large training data is available to capture the input-output trend over the entire design space, inverse modeling networks, conventional optimization methods combined with forward modeling networks, and GAN are suggested as suitable methods. Second, when the initial training set and the optimum are far apart in the vast design space, methodologies resolving the extrapolation challenge are introduced; gradual update of a machine learning model via the active transfer learning method, and devising an improved neural network architecture. Third, under the presence of two datasets with different fidelities, the domain transfer of an AI model using transfer learning was introduced. Finally, under the scarcity of data due to the objective function being too expensive to evaluate, we suggest a Bayesian optimization framework that makes efficient use of the data to determine the global optimum.

However, although many innovative AI model-based inverse design methods have emerged, there still remain challenges to be solved in order to more effectively utilize AI

models in manufacturing and materials design fields. First, it takes a lot of time to secure the initial training data used to build the AI surrogate model. In particular, to build the AI surrogate model for a problem with a large design space, at least a few thousand initial training data are required, and even after the data acquisition, the extrapolation challenge should also be considered in many cases. Physics-informed neural network (PINN) based methodology has been extensively explored recently to compensate for the lack of data and extrapolation challenge in solving the design problem [90, 91]. In addition, the quality of the data available in the manufacturing industry is still relatively low; most experimental data obtained in the field are unlabeled or noisy. In this review, the inverse design methodology based on supervised learning using labeled data has been mainly dealt with, but the semi-supervised training-based methodology that can utilize unlabeled data to create the surrogate model should be further investigated as a new route for data-driven inverse design methods [92, 93].

In conclusion, ML-based inverse design frameworks have become an innovative route for solving complex inverse design problems that were not handled before. However, it is crucial to choose the right algorithms according to the characteristics of the dataset and design space, and this review provides a concise guideline in the field of materials design and manufacturing. In the future, a design methodology that can exploit small, unlabeled, and noisy data sets should be further investigated to extend the impact of data-driven design methods in more practical engineering applications. At the same time, in addition to the development of algorithms, efforts to establish a database composed of standardized high-quality datasets should be paralleled.

Conflicts of interest

The authors declare no conflict of interest.

Acknowledgements

This work is financially supported by the National Research Foundation of Korea (NRF) (2022R1A2B5B02002365).

References

1. Mitchell, T.M. and T.M. Mitchell, *Machine learning*. Vol. 1. 1997: McGraw-hill New York.
2. Boulogeorgos, A.A.A., et al., *Machine learning in nano-scale biomedical engineering.* IEEE Transactions on Molecular, Biological and Multi-Scale Communications, 2020. **7**(1): p. 10-39.
3. Brunton, S.L., et al., *Data-driven aerospace engineering: reframing the industry with machine learning*. AIAA Journal, 2021. **59**(8): p. 2820-2847.
4. Brunton, S.L., B.R. Noack, and P. Koumoutsakos, *Machine learning for fluid mechanics.* Annual review of fluid mechanics, 2020. **52**: p. 477-508.
5. Dobbelaere, M.R., et al., *Machine learning in chemical engineering: strengths, weaknesses, opportunities, and threats.* Engineering, 2021. **7**(9): p. 1201-1211.
6. Ferguson, A.L., *Machine learning and data science in soft materials engineering.* Journal of Physics: Condensed Matter, 2017. **30**(4): p. 043002.
7. Guo, K., et al., *Artificial intelligence and machine learning in design of mechanical materials.* Materials Horizons, 2021. **8**(4): p. 1153-1172.
8. Hassanien, A.E., A. Darwish, and H. El-Askary, *Machine Learning and Data Mining in Aerospace Technology*. 2020: Springer.
9. Hosseini, M.-P., A. Hosseini, and K. Ahi, *A review on machine learning for EEG signal processing in bioengineering.* IEEE reviews in biomedical engineering, 2020. **14**: p. 204-218.
10. Jin, Z., et al., *Machine learning for advanced additive manufacturing.* Matter, 2020. **3**(5): p. 1541-1556.
11. Luo, F.-L., *Machine learning for future wireless communications.* 2020.
12. Nawaz, S.J., et al., *Quantum machine learning for 6G communication networks: State-of-the-art and vision for the future.* IEEE access, 2019. **7**: p. 46317-46350.
13. Yang, K.K., Z. Wu, and F.H. Arnold, *Machine-learning-guided directed evolution for protein engineering.* Nature methods, 2019. **16**(8): p. 687-694.
14. Zhong, S., et al., *Machine learning: new ideas and tools in environmental science and engineering.* Environmental Science & Technology, 2021. **55**(19): p. 12741-12754.
15. Jumper, J., et al., *Highly accurate protein structure prediction with AlphaFold.* Nature, 2021. **596**(7873): p. 583-589.
16. Silver, D., et al., *Mastering the game of go without human knowledge.* nature, 2017. **550**(7676): p. 354-359.
17. Omar, S., A. Ngadi, and H.H. Jebur, *Machine learning techniques for anomaly detection: an overview.* International Journal of Computer Applications, 2013. **79**(2).
18. Scime, L. and J. Beuth, *Anomaly detection and classification in a laser powder bed additive manufacturing process using a trained computer vision algorithm.* Additive Manufacturing, 2018. **19**: p. 114-126.
19. Escobar, C.A. and R. Morales-Menendez, *Machine learning techniques for quality control in high conformance manufacturing environment.* Advances in Mechanical Engineering, 2018.

10(2): p. 1687814018755519.

20. Peres, R.S., et al., *Multistage quality control using machine learning in the automotive industry.* IEEE Access, 2019. **7**: p. 79908-79916.
21. Tellaeche, A. and R. Arana. *Machine learning algorithms for quality control in plastic molding industry*. in *2013 IEEE 18th Conference on Emerging Technologies & Factory Automation (ETFA)*. 2013. IEEE.
22. Tiryaki, S. and A. Aydın, *An artificial neural network model for predicting compression strength of heat treated woods and comparison with a multiple linear regression model.* Construction and Building Materials, 2014. **62**: p. 102-108.
23. Khademi, F., et al., *Multiple linear regression, artificial neural network, and fuzzy logic prediction of 28 days compressive strength of concrete.* Frontiers of Structural and Civil Engineering, 2017. **11**(1): p. 90-99.
24. Yang, C., et al., *Using convolutional neural networks to predict composite properties beyond the elastic limit.* MRS Communications, 2019. **9**(2): p. 609-617.
25. Nie, Z., H. Jiang, and L.B. Kara, *Stress field prediction in cantilevered structures using convolutional neural networks.* Journal of Computing and Information Science in Engineering, 2020. **20**(1): p. 011002.
26. Reiner, J., R. Vaziri, and N. Zobeiry, *Machine learning assisted characterisation and simulation of compressive damage in composite laminates.* Composite Structures, 2021. **273**: p. 114290.
27. Pilania, G., et al., *Accelerating materials property predictions using machine learning.* Scientific reports, 2013. **3**(1): p. 1-6.
28. Sanchez-Lengeling, B. and A. Aspuru-Guzik, *Inverse molecular design using machine learning: Generative models for matter engineering.* Science, 2018. **361**(6400): p. 360-365.
29. Sun, H., H.V. Burton, and H. Huang, *Machine learning applications for building structural design and performance assessment: State-of-the-art review.* Journal of Building Engineering, 2021. **33**: p. 101816.
30. Zhou, Q., et al., *Property-oriented material design based on a data-driven machine learning technique.* The journal of physical chemistry letters, 2020. **11**(10): p. 3920-3927.
31. Weichert, D., et al., *A review of machine learning for the optimization of production processes.* The International Journal of Advanced Manufacturing Technology, 2019. **104**(5): p. 1889-1902.
32. Jeong, H., et al., *Phase field modeling of crack propagation under combined shear and tensile loading with hybrid formulation.* Computational Materials Science, 2018. **155**: p. 483-492.
33. Yang, C., et al., *Prediction of composite microstructure stress-strain curves using convolutional neural networks.* Materials & Design, 2020. **189**: p. 108509.
34. Wang, W., et al., *Machine learning prediction of mechanical properties of braided-textile reinforced tubular structures.* Materials & Design, 2021. **212**: p. 110181.
35. Pathan, M., et al., *Predictions of the mechanical properties of unidirectional fibre composites*

by supervised machine learning. Scientific reports, 2019. **9**(1): p. 1-10.

36. Gu, G.X., C.-T. Chen, and M.J. Buehler, *De novo composite design based on machine learning algorithm.* Extreme Mechanics Letters, 2018. **18**: p. 19-28.
37. Marcus, G., *Deep learning: A critical appraisal.* arXiv preprint arXiv:1801.00631, 2018.
38. Martius, G. and C.H. Lampert, *Extrapolation and learning equations.* arXiv preprint arXiv:1610.02995, 2016.
39. Barnard, E. and L. Wessels, *Extrapolation and interpolation in neural network classifiers.* IEEE Control Systems Magazine, 1992. **12**(5): p. 50-53.
40. Mitchell, J., et al., *Extrapolation in NLP.* arXiv preprint arXiv:1805.06648, 2018.
41. Greydanus, S., M. Dzamba, and J. Yosinski, *Hamiltonian neural networks.* Advances in neural information processing systems, 2019. **32**.
42. Long, Z., Y. Lu, and B. Dong, *PDE-Net 2.0: Learning PDEs from data with a numeric-symbolic hybrid deep network*. Journal of Computational Physics, 2019. **399**: p. 108925.
43. Kloss, A., S. Schaal, and J. Bohg, *Combining learned and analytical models for predicting action effects from sensory data.* The International Journal of Robotics Research, 2020: p. 0278364920954896.
44. Schmidhuber, J., *Deep learning in neural networks: An overview.* Neural networks, 2015. **61**: p. 85-117.
45. Whang, S.E., et al., *Data Collection and Quality Challenges in Deep Learning: A Data-Centric AI Perspective.* arXiv preprint arXiv:2112.06409, 2021.
46. Kim, Y., et al., *Designing an adhesive pillar shape with deep learning-based optimization.* ACS applied materials & interfaces, 2020. **12**(21): p. 24458-24465.
47. Yu, C.-H., et al., *End-to-End Deep Learning Model to Predict and Design Secondary Structure Content of Structural Proteins.* ACS Biomaterials Science & Engineering, 2022. **8**(3): p. 1156-1165.
48. Young, B.A., et al., *Can the compressive strength of concrete be estimated from knowledge of the mixture proportions?: New insights from statistical analysis and machine learning methods.* Cement and Concrete Research, 2019. **115**: p. 379-388.
49. Zhang, Z., et al., *Machine learning for accelerating the design process of double-double composite structures.* Composite Structures, 2022. **285**: p. 115233.
50. Hanakata, P.Z., et al., *Accelerated search and design of stretchable graphene kirigami using machine learning.* Physical review letters, 2018. **121**(25): p. 255304.
51. Kabir, H., et al., *Neural network inverse modeling and applications to microwave filter design.* IEEE Transactions on Microwave Theory and Techniques, 2008. **56**(4): p. 867-879.
52. Liu, D., et al., *Training deep neural networks for the inverse design of nanophotonic structures.* Acs Photonics, 2018. **5**(4): p. 1365-1369.
53. Jin, J., et al., *Deep neural network technique for high-dimensional microwave modeling and applications to parameter extraction of microwave filters.* IEEE Transactions on Microwave Theory and Techniques, 2019. **67**(10): p. 4140-4155.

54. Zhang, C., et al., *Multivalued neural network inverse modeling and applications to microwave filters.* IEEE Transactions on Microwave Theory and Techniques, 2018. **66**(8): p. 3781-3797.
55. Lew, A.J. and M.J. Buehler, *A deep learning augmented genetic algorithm approach to polycrystalline 2D material fracture discovery and design.* Applied Physics Reviews, 2021. **8**(4): p. 041414.
56. Zhang, W., et al., *Operating data-driven inverse design optimization for product usage personalization with an application to wheel loaders.* Journal of Industrial Information Integration, 2021. **23**: p. 100212.
57. Hecht-Nielsen, R., *Theory of the backpropagation neural network*, in *Neural networks for perception*. 1992, Elsevier. p. 65-93.
58. Peurifoy, J., et al., *Nanophotonic particle simulation and inverse design using artificial neural networks.* Science advances, 2018. **4**(6): p. eaar4206.
59. Goodfellow, I., et al., *Generative adversarial networks.* Communications of the ACM, 2020. **63**(11): p. 139-144.
60. Radford, A., L. Metz, and S. Chintala, *Unsupervised representation learning with deep convolutional generative adversarial networks.* arXiv preprint arXiv:1511.06434, 2015.
61. Ledig, C., et al. *Photo-realistic single image super-resolution using a generative adversarial network*. in *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2017.
62. Isola, P., et al. *Image-to-image translation with conditional adversarial networks*. in *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2017.
63. Kohl, S., et al., *Adversarial networks for the detection of aggressive prostate cancer.* arXiv preprint arXiv:1702.08014, 2017.
64. Hong, S.H., et al., *Molecular generative model based on an adversarially regularized autoencoder.* Journal of chemical information and modeling, 2019. **60**(1): p. 29-36.
65. Wang, K. and X. Wan. *Sentigan: Generating sentimental texts via mixture adversarial networks*. in *IJCAI*. 2018.
66. Yang, J., et al., *VocGAN: A high-fidelity real-time vocoder with a hierarchically-nested adversarial network.* arXiv preprint arXiv:2007.15256, 2020.
67. Mirza, M. and S. Osindero, *Conditional generative adversarial nets.* arXiv preprint arXiv:1411.1784, 2014.
68. Arjovsky, M., S. Chintala, and L. Bottou. *Wasserstein generative adversarial networks*. in *International conference on machine learning*. 2017. PMLR.
69. Kim, B., S. Lee, and J. Kim, *Inverse design of porous materials using artificial neural networks.* Science advances, 2020. **6**(1): p. eaax9324.
70. Yilmaz, E. and B. German. *Conditional generative adversarial network framework for airfoil inverse design*. in *AIAA aviation 2020 forum*. 2020.
71. Settles, B., *Active learning literature survey.* 2009.
72. Kim, Y., et al., *Deep learning framework for material design space exploration using active*

transfer learning and data augmentation. npj Computational Materials, 2021. **7**(1): p. 1-7.

73. Demeke, W., et al., *Neural network-assisted optimization of segmented thermoelectric power generators using active learning based on a genetic optimization algorithm.* Energy Reports, 2022. **8**: p. 6633-6644.
74. Lee, S., Z. Zhang, and G.X. Gu, *Generative machine learning algorithm for lattice structures with superior mechanical properties.* Materials Horizons, 2022. **9**(3): p. 952-960.
75. Chen, C.T. and G.X. Gu, *Generative deep neural networks for inverse materials design using backpropagation and active learning.* Advanced Science, 2020. **7**(5): p. 1902607.
76. Jung, J., et al., *Optimization of injection molding process using multi-objective bayesian optimization and constrained generative inverse design networks.* Journal of Intelligent Manufacturing, 2022: p. 1-14.
77. Park, D., et al., *A Generalizable and Interpretable Deep Supervised Neural Network to Predict Strain Field of Composite in Unseen Design Space.* Available at SSRN 4164581.
78. Yang, Z., C.-H. Yu, and M.J. Buehler, *Deep learning model to predict complex stress and strain fields in hierarchical composites.* Science Advances, 2021. **7**(15): p. eabd7416.
79. Pan, S.J. and Q. Yang, *A survey on transfer learning.* IEEE Transactions on knowledge and data engineering, 2009. **22**(10): p. 1345-1359.
80. Xu, Y., et al., *A method for predicting mechanical properties of composite microstructure with reduced dataset based on transfer learning.* Composite Structures, 2021. **275**: p. 114444.
81. Jung, J., et al., *Transfer learning for enhancing the homogenization-theory-based prediction of elasto-plastic response of particle/short fiber-reinforced composites.* Composite Structures, 2022. **285**: p. 115210.
82. Dong, R., et al., *Inverse design of composite metal oxide optical materials based on deep transfer learning and global optimization.* Computational Materials Science, 2021. **188**: p. 110166.
83. Jones, D.R., M. Schonlau, and W.J. Welch, *Efficient global optimization of expensive black-box functions.* Journal of Global optimization, 1998. **13**(4): p. 455-492.
84. Williams, C. and C. Rasmussen, *Gaussian processes for regression.* Advances in neural information processing systems, 1995. **8**.
85. Shahriari, B., et al., *Taking the human out of the loop: A review of Bayesian optimization.* Proceedings of the IEEE, 2015. **104**(1): p. 148-175.
86. Snoek, J., H. Larochelle, and R.P. Adams, *Practical bayesian optimization of machine learning algorithms.* Advances in neural information processing systems, 2012. **25**.
87. Park, K., et al., *Designing staggered platelet composite structure with Gaussian process regression based Bayesian optimization.* Composites Science and Technology, 2022. **220**: p. 109254.
88. Khan, N., D.E. Goldberg, and M. Pelikan. *Multi-objective Bayesian optimization algorithm*. in *Proceedings of the 4th Annual Conference on Genetic and Evolutionary Computation*. 2002. Citeseer.

89. Laumanns, M. and J. Ocenasek. *Bayesian optimization algorithms for multi-objective optimization*. in *International Conference on Parallel Problem Solving from Nature*. 2002. Springer.
90. Raissi, M., P. Perdikaris, and G.E. Karniadakis, *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations.* Journal of Computational physics, 2019. **378**: p. 686-707.
91. Lu, L., et al., *Physics-informed neural networks with hard constraints for inverse design.* SIAM Journal on Scientific Computing, 2021. **43**(6): p. B1105-B1132.
92. Chapelle, O., B. Scholkopf, and A. Zien, *Semi-supervised learning (chapelle, o. et al., eds.; 2006)[book reviews].* IEEE Transactions on Neural Networks, 2009. **20**(3): p. 542-542.
93. Guo, K. and M.J. Buehler, *A semi-supervised approach to architected materials design using graph neural networks.* Extreme Mechanics Letters, 2020. **41**: p. 101029.